

New model for system of mesoscopic Josephson contacts.

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, 142092, ., .

Quantum fluctuations of the phases of the order parameter in two - dimensional (2D) arrays of mesoscopic Josephson junctions and their effect on the destruction of superconductivity in the system are investigated by means of a quantum-cosine model that is free of the incorrect application of the phase operator. The proposed model employs trigonometric phase operators and makes it possible to study arrays of small superconducting granules, pores filled with superfluid helium, or Josephson junctions in which the average number of particles n_0 (effective bosons, He atoms, and so on) is small, and the standard approach employing the phase operator and the particle number operator as conjugate ones is inapplicable. There is a large difference in the phase diagrams between arrays of macroscopic and mesoscopic objects for $n_0 < 5$ and $U < J$ (U is the characteristic interaction energy of the particle per granule and J is the Josephson coupling constant). Reentrant superconductivity phenomena are discussed.

PACS: 73.23.Ps, 74.50.+r, 74.20.Mn

The development of microlithographic methods has now made it possible to produce regular arrays of extremely small metallic granules, Josephson junctions, and so on. The study of the properties of such objects is of interest not only from the fundamental standpoint but also in connection with their possible application in nanoelectronics. For this reason, a great deal of attention is now being devoted to the investigation of models reflecting the main properties of mesoscopic Josephson arrays (see Refs [1] - [9] and the literature cited therein).

In the present letter we call a granule (or a pore containing superfluid He) *mesoscopic* if the rms fluctuation of the number of effective bosons viz. "Cooper pairs" (or He atoms in a pore), are comparable to the average number of particles. We do not address the question of the character of the transition of an individual granule to the superconducting state (or helium in a pore to the superfluid state), making the assumption that this transition (or crossover) has already occurred at a higher temperature T_{c_0} and that the concept, which we employ below, of an effective boson (particle) is defined. In this connection we note only that, just as for nucleon pairing in nuclei, strictly speaking, there does not exist a critical size of granules in which pairing is possible (but, for example, the parity of the number of electrons, the character of the fillings of the levels, and so on are important). The exposition below concerns an array of mesoscopic superconducting granules, but the analysis can obviously be extended to the case of superfluid helium in a porous media.

In the present letter we show that the application of the phase and particle number operators as conjugate variables [1] ordinarily employed for describing such systems (in a quantum XY model) is limited to systems of *macroscopic* granules, while in the case of a small average number of particles per granule other models that do not employ the incorrect "phase operator" are required (see below). Recently, a boson Hubbard model that takes into account of not only quantum fluctuations of the phase, but also the modulus of the superconducting order parameters was used [7,8] to investigate the superconducting properties of an array of mesoscopic granules. However, it is of interest to examine a system in which the fluctuations of the local superfluid density on the granules are small even in the mesoscopic region, and the quantum fluctuations of the phases of the order parameter play the main role in the destruction of the global superconducting state of the array.

At temperatures below the temperature T_{c_0} at which superconductivity is established in an individual granule the state of the system is determined by two parameters [8,10]: a) the ratio of the characteristic Coulomb interaction energy $E_C \sim U/2$ of the particles in a granule with self - capacitance $C_0 = 4e^2/U$ and the Josephson energy for particles tunneling between granules $E_J \sim J$, the corresponding dimensionless quantum parameter being $q \equiv \sqrt{U/J}$, and 2) the dimensionless temperature of the system $T \equiv k_b T/J$.

1. The superconducting properties of an array of "macroscopic" superconducting granules have traditionally been investigated in a quantum XY model with the Hamiltonian

$$\hat{H}_{XY} = J \sum_{\langle i,j \rangle} (1 - \cos(\hat{\varphi}_i - \hat{\varphi}_j)) + \frac{U}{2} \sum_i (\hat{n}_i - n_0)^2 \quad (1)$$

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where the sum $\sum_{\langle i,j \rangle}$ in Eq.(1) extends over all nonrepeating pairs $\langle i,j \rangle$ of neighboring sites. The phases of the order parameter $\varphi_i \in [0, 2\pi)$ and the particle number operator \hat{n}_i in the i th granule is assumed, starting with Anderson's work [1] to be conjugate to the "phase operator" $\hat{\varphi}_i$: $\hat{n}_i - n_0 = \hat{\varphi}_i / \partial \varphi_i$. We note that the direct application of such a "phase operator" $\hat{\varphi}$ is, strictly speaking, incorrect, if for no other reason than that its effect is to transfer the state out of the domain of definition (the set of periodic $\psi(\varphi + 2\pi) = \psi(\varphi)$). Moreover, direct quantization of the order parameter as $\psi = \Delta e^{i\varphi} \rightarrow \hat{a} = \sqrt{\hat{n}} \hat{e}^{i\varphi}$ gives, in view of the boundness of the spectrum of the particle number operator $\hat{n} = \hat{a}^\dagger \hat{a}$, a nonunitary operator $\hat{e}^{i\varphi}$. This makes it impossible to introduce a hermitian phase operator and leads to many paradoxes [11].

Many such difficulties can be circumvented by considering the "trigonometric" operators $\widehat{\cos} \varphi$ and $\widehat{\sin} \varphi$ (which do not commute with each other), while leaving the phase operator $\hat{\varphi}$ itself undefined [12]. In this approach, all operators of physical quantities which are periodic functions of the phase (in terms of the quantum XY model) must be rewritten as sums of trigonometric functions, followed by the substitutions

$$\cos(\varphi) \rightarrow \widehat{\cos} \varphi = \frac{1}{2} \left(\hat{a}^\dagger \frac{1}{\sqrt{\hat{n}+1}} + \frac{1}{\sqrt{\hat{n}+1}} \hat{a} \right)$$

$$\sin(\varphi) \rightarrow \widehat{\sin} \varphi = \frac{i}{2} \left(\hat{a}^\dagger \frac{1}{\sqrt{\hat{n}+1}} - \frac{1}{\sqrt{\hat{n}+1}} \hat{a} \right)$$

where the operators \hat{a}^\dagger and \hat{a} are Bose particle creation and annihilation operators, and $\hat{n} = \hat{a}^\dagger \hat{a}$. As n_0 increases, when the rms fluctuations of the particle number in a granule are much smaller than their average value, the boundness of the spectrum of the operator \hat{n} becomes unimportant and the "quantum trigonometric operators" $\widehat{\cos} \varphi$ and $\widehat{\sin} \varphi$ introduced above transform into their quasiclassical limit $\cos(\varphi)$ and $\sin(\varphi)$.

Applying the procedure described above to the Hamiltonian (1) for our system, we have

$$\hat{H} = J \sum_{\langle i,j \rangle} \left(1 - \widehat{\cos} \varphi_i \widehat{\cos} \varphi_j - \widehat{\sin} \varphi_i \widehat{\sin} \varphi_j \right) + \frac{U}{2} \sum_i (\hat{n}_i - n_0)^2 \quad (2)$$

In what follows we shall, for brevity, refer to the model (2) as the *quantum cosine model*.

In the present letter we are interested in the system (2) with *integral* occupation numbers, when the average number of bosons in each granule $n_0 = \langle a_i^\dagger a_i \rangle$ is an *integer*. It can be shown (see Ref. [5] for an analysis of this case in the boson Hubbard model) that under this condition and at $T = 0$ the model (2) belongs to the same universality class as the quantum XY model (1). However, at *finite* temperatures the critical behavior of the quantum cosine model will be identical – in contrast to the system at zero temperature – to the critical behavior of the quantum XY model in some *finite* range of values of the average occupation number n_0 of the granules in the system (near integral values of n_0).

2. To calculate the properties of the system (2) in the plane of controlling parameters $\{q, T\}$, we used the quantum Monte Carlo method of integration along trajectories in a "checkerboard" modification [13], where the degrees of freedom of the discretized system are the occupation numbers $\{n_i^p\}$ of the sites of a three - dimensional lattice $N \times N \times 4P$ formed by $4P$ -fold multiplication of the initial $N \times N$ lattice along the imaginary - time axis.

In analyzing the superconducting properties of the array, attention was focused mainly on the analysis of the superfluid fraction (the analog of the "helicity modulus" in the quantum XY model; see Ref. [14]), the expression for which in terms of the quantum cosine model (2) has the form

$$\begin{aligned} \nu_s &= -\frac{1}{N^2} \langle \hat{T}_x \rangle - \frac{1}{N^2 T P} \sum_{\tau=0}^{P-1} \langle \hat{J}_x^{(p)}(\tau) \hat{J}_x^{(p)}(0) \rangle \\ \hat{T}_x &= -\sum_i \left(\widehat{\cos} \varphi_{i+x} \widehat{\cos} \varphi_i + \widehat{\sin} \varphi_{i+x} \widehat{\sin} \varphi_i \right), \\ \hat{J}_x^{(p)} &= \sum_i \left(\widehat{\sin} \varphi_{i+x} \widehat{\cos} \varphi_i - \widehat{\cos} \varphi_{i+x} \widehat{\sin} \varphi_i \right), \quad \hat{J}_x^{(p)}(\tau) = e^{\tau \beta \hat{H}/P} \hat{J}_x^{(p)} e^{-\tau \beta \hat{H}/P} \end{aligned} \quad (3)$$

The superfluid fraction was also found in terms of the fluctuation of the "winding number" [6,13].

An important quantity required for investigating the role of the mesoscopic nature of the system are the fluctuations of the particle number over the granule

$$\delta n^2 = \frac{1}{4PN^2} \left\langle \sum_{p=0}^{4P-1} \sum_i (n_i^p - n_0)^2 \right\rangle \quad (4)$$

3. Let us examine the Monte Carlo results for the quantum cosine model (2). The main quantity describing the state of the system at a given point $\{q, T\}$ of the phase diagram (Fig. 1) is the superfluid fraction ν_s . Vanishing of ν_s indicates disordering of the system. The measured curves of the superfluid fraction versus the temperature T for fixed values of quantum parameter q are presented in Fig. 2. This figure shows the computational results for a $N \times N$ 6×6 system with $n_0 = 1, 3, 5, 7$ and, for comparison, for the quantum XY model (1). For a weak interparticle interaction in the granules $q < 1$ (which in terms of the XY model corresponds to a small role of quantum fluctuations of the phase of the order parameter) the superconductor – metal transition temperature T_c depends strongly on the average number of particles n_0 in a granule (see Fig. 2a). The temperature $T_c(q)$ can be estimated from the universal relation $\nu_s(q; T_c) = 2T_c/\pi$ [14]. It is evident from the figure that to suppress fluctuation phenomena in a system of mesoscopic granules or pores requires *lower* temperatures than in the case of systems of macroscopic granules. As the particle density increases (transition to the case of an array of macroscopic granules), for $n_0 > 5$ the plots of $\nu_s(T; n_0)|_{q=const}$ merge, to within the limits of the measurement error, and the model (2) goes over to its limit – the quantum XY model. This observation is also confirmed in Fig. 3 which displays the dependence of the superfluid fraction in models (2) and (1) on the quantum parameter q at $T = 0.5$. We note that for $q > 1$ the properties of the models under study differ very little, and therefore the effect of the mesoscopicity of the granules in the array are very small. This is confirmed in Figure 2b.

An interesting effect which we found in our calculation is *re - entrant superconductivity* of an array of mesoscopic granules with respect to the parameter q (determining the characteristic particle interaction energy). The *increase* in the density of the superfluid component with increasing quantum parameter q at a fixed temperature T , clearly seen in Fig. 3, is confirmed by computational results for the model (2) in mean field theory [15] (see Fig. 1).

The phase diagram of an ordered two-dimensional Josephson array of mesoscopic granules was constructed using the results presented above (see Fig. 1). For comparison, the computational results obtained in mean field theory, which is in qualitative agreement with the Monte Carlo data, is also shown. We note, for comparison, that taking the fluctuations of the modulus of the order parameter (local superfluid density) into account in the boson Hubbard model *increases* the superconducting transition temperature of a mesoscopic system [8].

The character of the phase transition occurring along the line $T_c(q)$ can be analyzed in greater detail by studying the fluctuations of the particle number over the granules (4) as a function of the temperature and quantum parameter. The calculations show that as the temperature increases, the fluctuations of the particle number over the granules increases, as is characteristic for a transition to a state with a higher conductivity. Therefore, at finite temperatures the line of phase transitions $T_c(q)$ (see Fig. 1) is a line of superconductor - to - metal transitions. Conversely, at a fixed temperature the particle- number fluctuations $\delta n^2(q)$ as a function of the quantum parameter q decrease, as is characteristic for a (finite - temperature crossover) transition to a Mott insulator state [16].

From the relative rms particle - number fluctuations $\epsilon_n \equiv \sqrt{\delta n^2/n_0^2}$ it can be concluded that the value $\epsilon = \epsilon_n^{mes} \sim 0.5$ can be regarded as a criterion for determining the mesoscopicity of granules in the array, namely, for smaller relative fluctuations the system can be viewed as consisting of macroscopic granules and can be described by the quantum XY model (1).

4. Thus, a new model has been proposed for systems of mesoscopic Josephson junctions - the quantum cosine model (2), which takes into account the quantum fluctuations of the phases of the order parameter and does *not* employ an incorrect definition of the "phase operator". This model can be used to investigate the properties of systems of mesoscopic granules or pores containing a superfluid *He*, where the relative fluctuation of the "effective bosons" over the granules or atoms of the liquid in the pores are large and the quantum XY model (1) is inapplicable.

The computational results show that in the case of a system of weakly interacting particles (for $q < 1$) the temperature at which a global superconducting state appears depends strongly on the particle density, approaching *from below* the metal - superconductor transition temperature in a system of macroscopic granules or pores. It was found that the corresponding "macroscopic" limit, where the system is adequately described in a quantum XY model (1), is reached at comparatively low densities, $n_0 \sim 5$.

In the region of large quantum fluctuations of the phases ($q > 1$), the relative fluctuations of the particle number over the granules are strongly suppressed by the interaction, and mesoscopic effects are important only at low temperatures ($T < 0.5$) and low densities ($n_0 \sim 1$).

As one can see from the results of calculations, the proposed quantum cosine model (2) does not (at least in the investigated range of the controlling parameters) exhibit re-entrant superconductivity with respect to *temperature*, where for some values of the quantum parameter q a global superconducting state is absent at both high and low temperatures. However, for a weak interparticle interaction, when $q < 1$, there is re-entrant superconductivity with

respect to the *quantum parameter* q . We found that for the model (1), in contrast to the behavior of the Hubbard model and the quantum XY model, the degree of disorder in the system increases with increasing interaction of the bosons (with decreasing strength of quantum fluctuations of the phases in terms of the quantum XY model).

We thank V.F. Gantmakher for a helpful discussion of the results of this work. This work was supported by grants from the Russian Fund for Fundamental Research and the programs "Physics of Solid-State Nanostructures" and "Surface Atomic Structures".

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Fig. 1

Phase diagrams of the quantum, cosine model (QC), the boson Hubbard model (H) [8], and the quantum XY model (2+1 XY) [17]. S - superconducting state, N - normal state.

Insert: Mean field theory results [15]: **1** - $n_0 = 1$; **2** - $n_0 = 2$; **3** - $n_0 = 6$; **4** - quantum XY model ($n_0 = \infty$);

Here and below the symbols represent the quantum Monte Carlo results: open symbols - $N = 10$, filled symbols - $N = 6$, squares - $n_0 = 1$, circles - $n_0 = 3$, triangles - $n_0 = 5$, rhombi - $n_0 = 7$, asterisks - quantum XY model.

Fig. 2

Superfluid fraction ν_s (helicity modulus γ in the case of quantum XY model) versus temperature T : **a**) $q = 0.2$; **b**) $q = 2.0$; The dotted line shows the curve $2T/\pi$. A spline interpolation is drawn in as an aid to the eye. The statistical errors, which are not shown, are less than the size of the corresponding symbols.

Fig. 3

Superfluid fraction ν_s (helicity modulus γ in the case of quantum XY model) versus the quantum parameter q at $T = 0.5$; the dotted line shows the line $1/\pi$. Insert: $\nu_s(q)$ at $T = 1$.

Translated by M.E. Alferieff.





